Managing and Accessing Large Scientific Datasets

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Outline

• What are scientific data
• Describing and storing it
• Access it
• Cross-project collections
What are scientific data?
What are scientific data?

- A variety of data types and structures
- Large data structures
- Many objects
- Metadata: parameters, variables, legacy in a variety of forms
Requirements for Scientific Data

- Portability/sharability
  - Access software works on many machines
  - Applications can understand all relevant data
  - Data accessible on many machines
  - Sharable data across applications
  - Open standards

- Efficient storage and access
- Extensibility
- Software support
New challenges

• Bigger, faster machines and storage systems
  – massive parallelism, teraflop speeds
  – parallel file systems, terabyte storage

• Greater complexity
  – complex data structures
  – complex subsetting

• Remote and distributed access

• Legacy data
Describing and organizing scientific data
### Abstraction Layers

**Information for describing data exists at many levels**

<table>
<thead>
<tr>
<th>Layer</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Feature/object</strong></td>
<td>Image, data point, <em>ERP component</em>?</td>
</tr>
<tr>
<td><strong>Science data model</strong></td>
<td>Geometry, variable, field</td>
</tr>
<tr>
<td><strong>Data structures</strong></td>
<td>Array, mesh, index</td>
</tr>
<tr>
<td><strong>Datatypes</strong></td>
<td>Integer, string</td>
</tr>
<tr>
<td><strong>Physical format</strong></td>
<td>ASCII text, native binary, IEEE</td>
</tr>
<tr>
<td><strong>Storage model</strong></td>
<td>Raw file, collection, database</td>
</tr>
</tbody>
</table>
Science data models

• Data
  – Independent variables
  – Dependent variables, fields

• Context
  – Parameters
  – Spatiotemporal context -- topology, geometry, time
  – Relationships and dynamics
  – Provenance
Data structures

- Simple aggregates (array, table)
- Compound aggregates
  - Grid (regular, irregular, multi-resolution)
  - Sequence of records (extendable table/array)
  - Random access structure (hash table, tree)
  - Index structures (multi-view, random access)
  - Other aggregates (list, stack, queue)
- Other organizational structures
  - groups
  - attributes
See “Terra’s Orbit” at http://terra.nasa.gov/Gallery/browse.php3 for an animation that illustrates a swath.
See “MOPITT Scanning Swath” at http://terra.nasa.gov/Gallery/browse.php3 for an animation that illustrates a mopitt swath.
See “MODIS Scanning Swath” at http://terra.nasa.gov/Gallery/browse.php3 for an animation that illustrates a modis swath.
See “Combined Swaths” at http://terra.nasa.gov/Gallery/browse.php3 for an animation illustrating swath all.
HDF-EOS Swath

Data fields

“Brightness Temperature”

Map1
DataDimension: “Track”
Geodimension: “Geotrack”
Offset: 1
Increment: 2

Dimension
Name: Track
Size: 42

Dimension
Name: Scan
Size: 16

Dimension
Name: Geotrack
Size: 21

Geolocation fields

“Time”

“Latitude”

“Longitude”
Datatypes

- Standard integer & float
- User-definable scalars (e.g. 13-bit integer)
- Variable length types (e.g. strings)
- Pointers - references to objects/regions
- Enumeration - nominal
- Compound types (records)
Physical organization

• File formats
  – Standard formats
  – Home-grown
  – Questions of simplicity
  – Files need not be files
Files need not be files

A file handle accesses storage through one or more layers of low-level file drivers.
Physical organization

• Storage options
  – Text vs. binary
  – Self-describing vs simple
  – Random vs. sequential access
  – Storage structures
Interesting Storage Options

- **Chunked array**
  - Better subsetting access time; extendable

- **compressed**
  - Improves storage efficiency, transmission speed

- **extendable**
  - Supports record view

- **split file**
  - Metadata in one file, raw data in another.

Dataset “Fred”

File A

File B

Data for Fred

Metadata for Fred
Example of layers: ASCI DMF

- Objectives
  - Sound data model with robust data abstractions
  - Computational mechanics data: meshes & fields
  - Based on mathematical field of fiber bundles
  - Common format allows common tools & sharing
  - Common API shield apps from model complexities
Accessing Scientific Data
Accessing scientific data

- Partial access
  - When you only want part of the data
  - When you don't have enough space
  - When you don't have enough time

- Transformations
  - Data types
  - Data objects at all levels
    - mesh --> image
    - subsetting
(a) A hyperslab from one 2D array to corner of another 2D array

(b) A regular series of blocks from a 2D array to a contiguous sequence at a certain offset in a 1D array

(c) A sequence of points from a 2D array to a sequence of points in a 3D array.

(d) Union of hyperslabs in file to union of hyperslabs in memory. Number of elements must be equal.
Accessing scientific data

- Indirect access
  - index or other structure points to data
- Fusion
  - combining two or more datasets to produce another dataset
- Remote vs. local
- Parallel access
Cross-project collections

• Can be organized (or not) in many ways
• Ad hoc
  – Each research team does its own thing
  – Individual files and formats
• Database
  – Single schema fits all
  – Or distributed DB
• Federation
  – Different collections, common semantics
  – Common format, or objects
**EOSDIS Processing Levels**

- **Level 0**: Raw instrument data time ordered, duplications removed, original restored
- **Level 1A**: Radiometrically Corrected
  - Reversibly transformed L0 data, located to coordinate system + Ancillary + Engineering
- **Level 1B**: Environmental variables, same location as L1
- **Level 3**: Data or environmental variables, spatial and/or temporal resampling
- **Level 4**: Model output
## EOSDIS Example: Library Analogy

<table>
<thead>
<tr>
<th>EOSDIS</th>
<th>LIBRARY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granule</td>
<td>Granule Metadata</td>
</tr>
<tr>
<td>Book</td>
<td>Index Card</td>
</tr>
<tr>
<td>Collection</td>
<td>Collection Metadata</td>
</tr>
<tr>
<td>Book Collection</td>
<td>Collection Indexing</td>
</tr>
<tr>
<td>Catalogue</td>
<td>Catalogue Interoperability Protocol</td>
</tr>
<tr>
<td>Catalogue</td>
<td>Catalogue Indexing</td>
</tr>
</tbody>
</table>
## Example Categories for Granule- and Collection-Level Metadata

<table>
<thead>
<tr>
<th>Granule</th>
<th>Collection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Platform, Instrument, Sensor</td>
<td>Platform, Instrument, Sensor</td>
</tr>
<tr>
<td>Spatial and Temporal</td>
<td>Delivered Algorithm Package</td>
</tr>
<tr>
<td>Orbit Parameters</td>
<td>Guide</td>
</tr>
<tr>
<td>Browse</td>
<td>Bibliographic Reference</td>
</tr>
<tr>
<td>QA Data Statistics</td>
<td>Papers/Documents</td>
</tr>
<tr>
<td>Production History</td>
<td>Keyword</td>
</tr>
</tbody>
</table>
Object Based
Digital Library Architecture

User Interface

Meta-data query

Result documents

Meta-data manipulation services

DL Middleware

Data object (text,image)

Request for data (X.509)

Data Handling System

Archive HPSS

Searchable Metadata
(fields from XML/SGML)
SDSC Storage Resource Broker & Meta-data Catalog

MCAT

Resource

User

Dublin Core

Application Meta-data

Application

File SID

DBLobj SID

Obj SID

SRB

ADSM

HPSS

DB2

Oracle

Unix
Thank you